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STN STRUCTURE SEARCH (REGISTRY/CAPLUS)

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 02	STN pricing information for 2008 now available
NEWS 3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 5	JAN 28	MARPAT searching enhanced
NEWS 6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS 9	FEB 08	STN Express, Version 8.3, now available
NEWS 10	FEB 20	PCI now available as a replacement to DPCI
NEWS 11	FEB 25	IFIREF reloaded with enhancements
NEWS 12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS 16	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS 17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS 18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS 20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS 22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS 23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS 24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 28	JUN 19	CAS REGISTRY includes selected substances from web-based collections

```
 NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:19:21 ON 24 JUN 2008

=> FIL REG
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 17:19:37 ON 24 JUN 2008
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COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   23 JUN 2008  HIGHEST RN 1030103-54-8
DICTIONARY FILE UPDATES:  23 JUN 2008  HIGHEST RN 1030103-54-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\Jan1.str
```
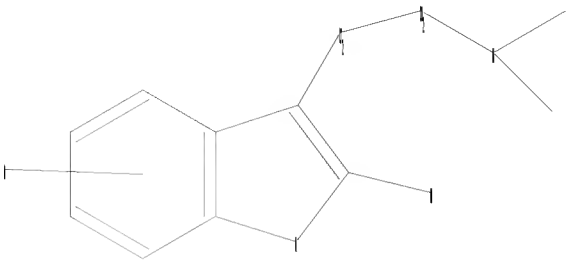
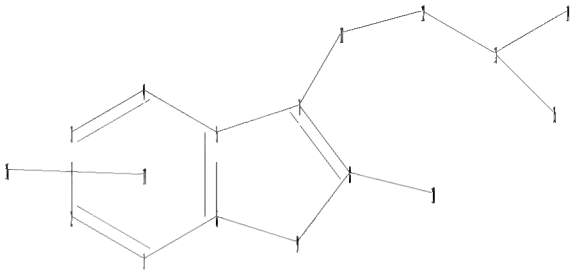



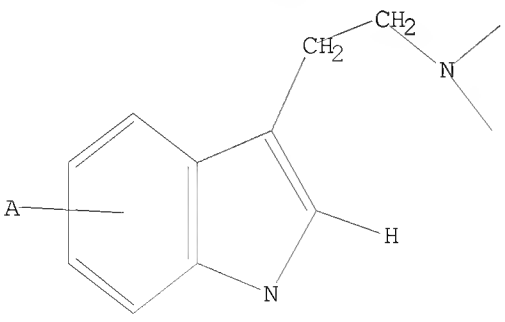


chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L1 STRUCTURE UPLOADED

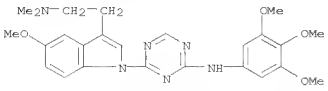
=> D
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> S L1
SAMPLE SEARCH INITIATED 17:19:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    18996 TO ITERATE

 10.5% PROCESSED     2000 ITERATIONS                                35 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       371667 TO   388173
PROJECTED ANSWERS:            5555 TO     7741

L2           35 SEA SSS SAM L1

=> D SCAN
```

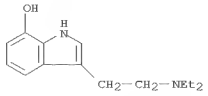
L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1H-Indole-3-ethanamine, 5-methoxy-N,N-dimethyl-1-[4-[(3,4,5-trimethoxyphenyl)amino]-1,3,5-triazin-2-yl]-
MF C25 H30 N6 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1H-Indol-7-ol, 3-[2-(diethylamino)ethyl]-
MF C14 H20 N2 O

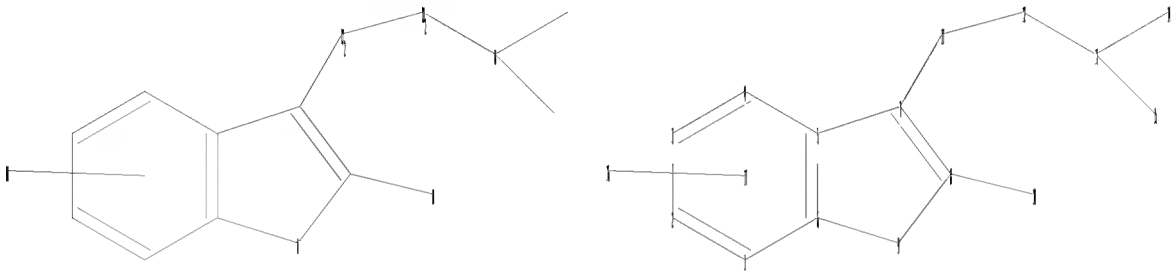


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

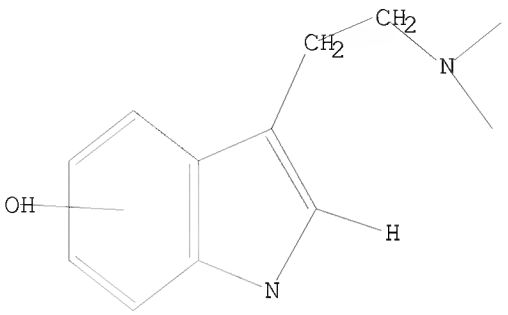
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```
=> S L1 FULL
FULL SEARCH INITIATED 17:20:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   377430 TO ITERATE

100.0% PROCESSED   377430 ITERATIONS                                6038 ANSWERS
SEARCH TIME: 00.00.02

L3         6038 SEA SSS FUL L1
```

```
=>
Uploading C:\Program Files\Stnexp\Queries\10539151\JUNE1.str
```



```
chain nodes :
10  11  12  16
ring nodes :
1  2  3  4  5  6  7  8  9
ring/chain nodes :
13  14  15
chain bonds :
7-11  8-10  11-12  12-13
ring/chain bonds :
13-14  13-15
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  13-14  13-15
exact bonds :
7-11  8-10  11-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:Atom



L4      STRUCTURE UPLOADED

=> D
L4 HAS NO ANSWERS
L4              STR
```



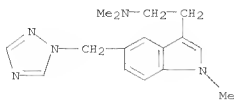
Structure attributes must be viewed using STN Express query preparation.

```
=> S L4 FULL SUB=L3
FULL SUBSET SEARCH INITIATED 17:21:28 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -     6038 TO ITERATE

100.0% PROCESSED     6038 ITERATIONS                              275 ANSWERS
SEARCH TIME: 00.00.01

L5          275 SEA SUB=L3 SSS FUL L4

=> S L3 NOT L5
L6         5763 L3 NOT L5
```

=> D SCAN

L6 5763 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1H-Indole-3-ethanamine, N,N,1-trimethyl-5-(1H-1,2,4-triazol-1-ylmethyl)-, ethanedioate (1:1)
MF C16 H21 N5 . C2 H2 O4

CM 1

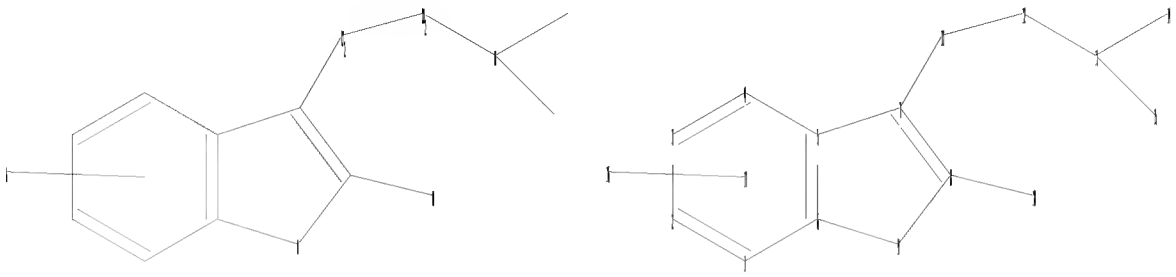


CM 2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\JUNE2.str

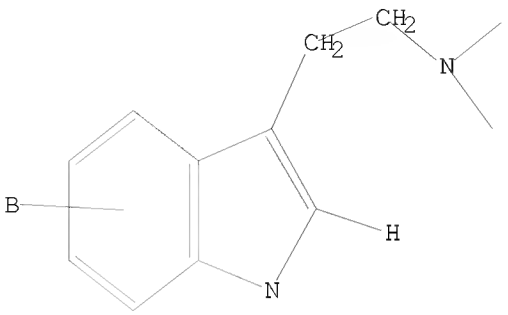


chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

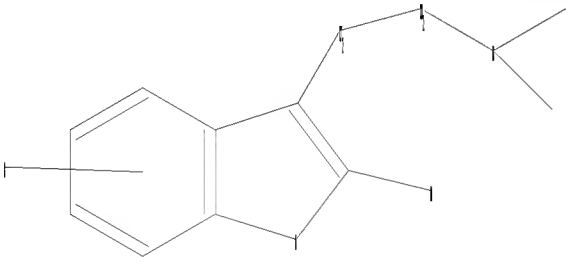
L7 STRUCTURE UPLOADED

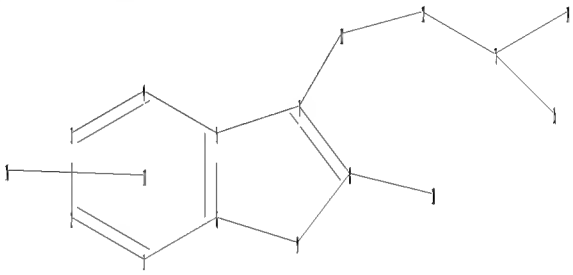
=> D
L7 HAS NO ANSWERS
L7 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> S L7 FULL SUB=L6
FULL SUBSET SEARCH INITIATED 17:23:05 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -        9 TO ITERATE

100.0% PROCESSED        9 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L8             0 SEA SUB=L6 SSS FUL L7

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\JUNE3.str
```





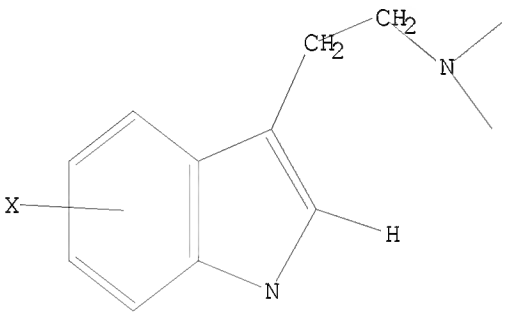
```
chain nodes :
10  11  12  16
ring nodes :
1  2  3  4  5  6  7  8  9
ring/chain nodes :
13  14  15
chain bonds :
7-11  8-10  11-12  12-13
ring/chain bonds :
13-14  13-15
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  13-14  13-15
```

exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L9 STRUCTURE UPLOADED

=> D
L9 HAS NO ANSWERS
L9 STR



Structure attributes must be viewed using STN Express query preparation.

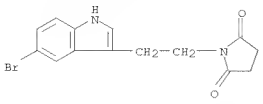
=> S L9 FULL SUB=L6
FULL SUBSET SEARCH INITIATED 17:24:10 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 5763 TO ITERATE

100.0% PROCESSED 5763 ITERATIONS 1320 ANSWERS
SEARCH TIME: 00.00.01

L10 1320 SEA SUB=L6 SSS FUL L9

=> D SCAN

L10 1320 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,5-Pyrrolidinedione, 1-[2-(5-bromo-1H-indol-3-yl)ethyl]-
MF C14 H13 Br N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```
=> FIL CAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   307.88     308.09

FILE 'CAPLUS' ENTERED AT 17:24:22 ON 24 JUN 2008
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FILE COVERS 1907 - 24 Jun 2008  VOL 148 ISS 26
FILE LAST UPDATED: 23 Jun 2008  (20080623/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> S L10
L11        229 L10

=> D IBIB ABS HITSTR 229
```

L11 ANSWER 229 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN

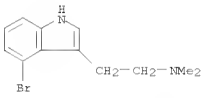
ACCESSION NUMBER: 1957:66823 CAPLUS
DOCUMENT NUMBER: 51:66823
ORIGINAL REFERENCE NO.: 51:12147c-d
TITLE: Indole and homologs
PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1135022		19570423	FR	19551029
DE 1082265			DE	

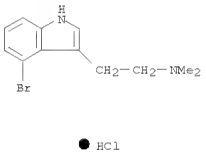
AB A substituted formamidine is heated in the presence of a alkaline alcoholate in a solvent of the same alc. as the alcoholate used and, eventually, the amine corresponding to the formamidine at about 220-50°, the amine and alc. distilled giving the indole as residue.

IT 28289-22-7 108992-10-5
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 28289-22-7 CAPLUS
CN 1H-Indole-3-ethanamine, 4-bromo-N,N-dimethyl- (CA INDEX NAME)



RN 108992-10-5 CAPLUS
CN Indole, 4-bromo-3-(2-dimethylaminoethyl)-, hydrochloride (6CI) (CA INDEX NAME)



L11 ANSWER 229 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L11 ANSWER 228 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:66824 CAPLUS
DOCUMENT NUMBER: 51:66824
ORIGINAL REFERENCE NO.: 51:12147d-g
TITLE: 5-Chloro(or bromo)-2-methyl-3-(N-substituted-amino-methyl)indoles
PATENT ASSIGNEE(S): Farmaceutici Italia SA
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

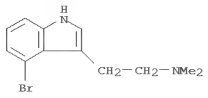
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 773440		19540703	GB	
DE 1079641			DE	

AB Products possessing an antagonistic action to 5-hydroxytryptamine for the control of morbid syndroms resulting from an excess of this substance, are synthesized by (1) preparing the starting material, 5-chloro(or bromo)-2-methylindole and (2) treating it with a secondary amine. Thus, 15 ml. H_2O, 5 ml. acetone, and 5 ml. saturated aqueous NaOAc are added to 6 g. p-bromophenylhydrazine-HCl, 25 ml. ether added in an N atmospheric, the ether layer dried with $CaCl_2$, transferred to a small flask with 30 g. anhydrous $ZnCl_2$, heated slowly in N atmospheric using an oil bath in order to evaporate the solvent, then the temperature raised to 150° for a few min. The mixture is cooled, H_2O and HCl are added, then steam-distilled to give 5-bromo-2-methylindole, m. 93-6°. Glacial AcOH (25 ml.) and 14.5 ml. 55% aqueous MeNH are mixed slowly at 0° with 13 ml. 38% H_2CO, then poured on to a mixture of 25 g. 5-chloro-2-methylindole, stirred to dissolve, left 6 hrs., then poured into 500 ml. 5% NaOH and kept at 0° 2 hrs. The separated product is filtered off, dissolved in ether, dried with Na_2SO_4, acetone added; after evaporation about 22 g. 5-chloro-2-methyl-3-(N-dimethylaminomethyl)indole, m. 157-9° (from MeOH), is obtained; HCl salt, m. 177-9° (from alc.). The 5-Br analog m. 143-5° (from ether-acetone). When piperidine was used as the secondary amine, 5-chloro-2-methyl-3-piperidinomethylindole was obtained, m. 161-3° (from MeOH or C_6H_6).

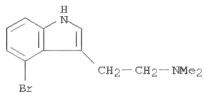
IT 28289-22-7 108992-10-5
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 28289-22-7 CAPLUS
CN 1H-Indole-3-ethanamine, 4-bromo-N,N-dimethyl- (CA INDEX NAME)

L11 ANSWER 228 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 108992-10-5 CAPLUS
CN Indole, 4-bromo-3-(2-dimethylaminoethyl)-, hydrochloride (6CI) (CA INDEX NAME)

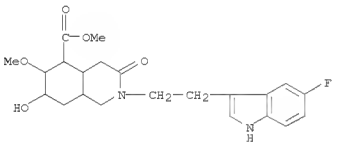


● HCl

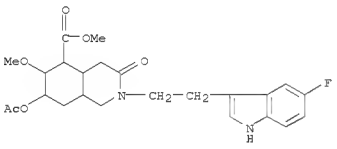
L11 ANSWER 227 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:34370 CAPLUS
DOCUMENT NUMBER: 54:34370
ORIGINAL REFERENCE NO.: 54:6775c-h
TITLE: Antihypertensive agents. II. Tropine quaternaries
AUTHOR(S): Shapiro, Seymour L.; Soloway, Harold; Freedman, Louis
CORPORATE SOURCE: U.S. Vitamin & Pharm. Corp., Yonkers, NY
SOURCE: Journal of Organic Chemistry (1959), 24, 1607-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 52, 18396h. A series of tropine (I) quaternary salts were prepared for pharmacol. screening. Synthesis was effected by treating a mixture of the quaternizing halide with I in a polar solvent. I (5.6 g.) and 5.3 g. CH2I2 in 30 ml. MeCN kept 5 days at 20° gave 5 g. N-(iodomethyl)tropinium iodide. The same compound was obtained from a 1:1 molar ratio of the reactants at 20°, or when the reaction mixture was refluxed 0.5 hr. The reaction of I with pentaerythrityl tetrabromide failed with no evidence of quaternization after 50 hrs. refluxing with MeCN. I (4.2 g.), 5.6 g. α-chloroacetamide, and 60 ml. MeCN kept 5 days at 20° gave 4.7 g. N-(carbamoylmethyl)tropinium chloride. An addnl. 1.4 g. was obtained by adding Et2O to the filtrate. The following preparation was typical of the synthesis of compds. of the α-haloacetamides. N-Methylaniline (11.8 g.) in 75 ml. MeCN added slowly to 5.7 g. ClCH2COCl in 25 ml. MeCN, left 48 hrs. at 20°, the N-methylaniline-HCl removed, and the filtrate evaporated gave 8.8 g. N-methyl-α-chloroacetanilide. The consts. of most of the α-haloacetamides were in agreement with reported values. The following were new compds.: N-benzyl-N-isopropylbromoacetamide, b0.2 124-36°; N-(α-phenylethyl)bromoacetamide, m. 82-3° (hexane); N-[(2,5-endomethylenecyclohexyl)methyl]bromoacetamide, b0.04 104-30°. The following compds. were thus prepared [R of TrRNX (TrN = tropine), X, m.p., recrystn. solvent, and % yield given]: C12H25, Br, 211-13°, alc.-isopropyl ether, 58; 2-cyclohexylethyl, Br, 182-5°, isopropyl ether-iso-PrOH, 49; Ph(CH2)3, Br, 217-20°, alc., 84; Ph2CH, Cl, 195-7°, alc., 9; HC.tplbond.CCH2, Br, 243-5°, alc., 57; ICH2, I, 203-6°, MeOH, 31; IC.tplbond.CCH2, Cl, 212°, alc., 12; (CH2)2NEt2.HCl, Cl, above 300°, alc., 32; CH2CH:CHCH2 (di-salt), 2Cl, above 300°, MeOH, 37; CH2C.tplbond.CCH2 (di-salt), 2Cl, 260-3°, alc., 21; (CH2)5 (di-salt), 2Br, above 300°, MeOH, 30; (CH2)6 (di-salt), 2Br, 282-5°, isopropyl ether-MeOH, 22; AcCH2, Cl, 246-7°, iso-PrOH, 47; BzCH2, Cl, 220-3°, iso-PrOH, 41. For compds. where R = R1R2NCOCH2, R1, R2, X, m.p., recrystn. solvent, and % yield were given: H, H, Cl, 258-60°, alc., 58; Me, Me, Br, 242-3°, MeCN, 57; (CH2)4, Br, 241°, alc., 61; iso-C5H11, H, Cl, 183-4°, Et2O, 33; (2,5-endomethylenecyclohexyl)methyl, H, Br, 246-8°, iso-PrOH-hexane, 52; PhCH2, H, Cl, 196-7°, MeCN, 32; PhCHMe, H, Br, 198-9°, iso-PrOH-hexane, 47; PhCH2, iso-Pr, Br, 169-72°, hexane-Et2O, 35; PhCH2CHMe, H, Cl, 204-7°, EtOAc, 49; Ph, H, Cl, 175-8°, iso-PrOH, 39; p-ClC6H4, H, Cl, 247-8°, iso-PrOH, 44. All of the compds. were evaluated for hypotensive response. In the

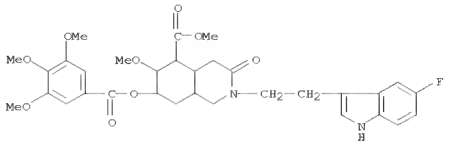
L11 ANSWER 227 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 96456-41-6 CAPLUS
CN 5-Isoquinolinecarboxylic acid, 2-[2-(5-fluoroindol-3-yl)ethyl]decahydro-7-hydroxy-6-methoxy-3-oxo-, methyl ester, acetate (6CI, 7CI) (CA INDEX NAME)

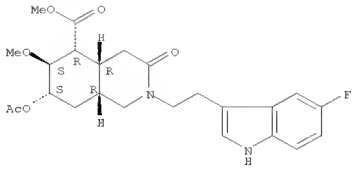


L11 ANSWER 227 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
carbamoyl series the hypotensive activity was assocd. with the compds. where R1 R2 = H, and R1 = aralkyl or aryl and R2 = H.
IT 2267-06-3 3829-05-8 3910-74-5
96456-41-6
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 2267-06-3 CAPLUS
CN 5-Isoquinolinecarboxylic acid, 2-[2-(5-fluoro-1H-indol-3-yl)ethyl]decahydro-6-methoxy-3-oxo-7-[(3,4,5-trimethoxybenzoyl)oxy]-, methyl ester (CA INDEX NAME)



RN 3829-05-8 CAPLUS
CN 5-Isoquinolinecarboxylic acid, 7-(acetyloxy)-2-[2-(5-fluoro-1H-indol-3-yl)ethyl]decahydro-6-methoxy-3-oxo-, methyl ester, (4aα,5β,6α,7β,8aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



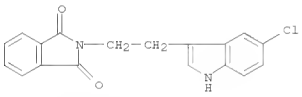
RN 3910-74-5 CAPLUS
CN 5-Isoquinolinecarboxylic acid, 2-[2-(5-fluoroindol-3-yl)ethyl]decahydro-7-hydroxy-6-methoxy-3-oxo-, methyl ester (6CI, 7CI, 8CI) (CA INDEX NAME)

L11 ANSWER 100 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:386898 CAPLUS
DOCUMENT NUMBER: 127:95163
ORIGINAL REFERENCE NO.: 127:18321a,18324a
TITLE: Synthesis of 2-aryltryptamines with palladium catalyzed cross-coupling of 2-bromotryptamines and arylboronic acids
AUTHOR(S): Chu, Lin; Fisher, Michael H.; Goulet, Mark T.; Wyvratt, Matthew J.
CORPORATE SOURCE: Dep. Med. Chem., Merck Research Lab., Rahway, NJ, 07065, USA
SOURCE: Tetrahedron Letters (1997), 38(22), 3871-3874
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:95163

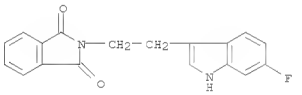
AB A versatile and high-yielding synthesis of 2-aryltryptamines employing palladium(0) catalyzed cross-coupling of 2-bromotryptamines and arylboronic acids was developed. The preparation of the intermediate 2-bromotryptamines with pyridine hydrobromide perbromide as the brominating agent, is also reported.

IT 55747-68-7P 192182-60-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryltryptamines by palladium catalyzed cross-coupling of
2-bromotryptamines with arylboronic acids)

RN 55747-68-7 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[2-(5-chloro-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



RN 192182-60-8 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[2-(6-fluoro-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



L11 ANSWER 100 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L11 ANSWER 101 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:234030 CAPLUS
DOCUMENT NUMBER: 126:338782
ORIGINAL REFERENCE NO.: 126:65731a,65734a
TITLE: Simultaneous measurement of [3H]noradrenaline release and neurogenic contraction under identical conditions, to determine the prejunctional inhibitory effects of SKF 99101H and BRL 56905 in dog saphenous vein
AUTHOR(S): Medhurst, Andrew D.; Brown, Antony M.; Kaumann, Alberto J.; Parsons, Andrew A.
CORPORATE SOURCE: Department Neurology Research, SmithKline Beecham Pharmaceuticals, Harlow, CM19 5AW, UK
SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1997), 355(4), 475-482
CODEN: NSAPCC; ISSN: 0028-1298
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Using a tissue bath system which allowed the simultaneous measurement of elec.-induced [3H]noradrenaline release and neurogenic contraction under identical conditions, we investigated the prejunctional inhibitory activity of the selective 5-HT1D/1B receptor agonists BRL 56905 ((±)-3-amino-6-carboxamido-1,2,3,4-tetrahydrocarbazole) and SKF 99101H (3-(2-dimethylaminoethyl)-4-chloro-5-propoxyindole hemifumarate), compared to sumatriptan and 5-HT. Transmural elec. stimulation (2 Hz) of dog saphenous vein induced consistent increases in [3H]noradrenaline release as well as reproducible contractile responses (< 10% decrease over four stimulation periods). BRL 56905, SKF 99101H, sumatriptan and 5-HT (60 nM-6 μM) inhibited elec.-evoked [3H]noradrenaline release and neurogenic contractile responses in dog saphenous vein. However, despite being measured under identical conditions, the inhibition of [3H]noradrenaline release was consistently greater than the inhibition of neurogenic contraction induced by a particular concentration of agonist, suggesting that neurogenic contractile responses in dog saphenous vein result from the combined release of noradrenaline and other non-noradrenergic neurotransmitters. Under the present assay conditions, since the agonists produced only small (BRL 56905, sumatriptan and 5-HT) or marginal (SKF 99101H) contractile responses, it is unlikely that this is the cause of the discrepancy observed between inhibition of release and inhibition of contraction. The inhibitory effects of BRL 56905, sumatriptan and 5-HT were blocked by the 5-HT1D/1B receptor antagonist methiothepin, consistent with the involvement of canine ca-5-HT1D/1B receptors in inhibiting neurotransmitter release and subsequent smooth muscle contraction in dog saphenous vein. The present results show that the novel 5-HT1D/1B receptor agonists BRL 56905 and SKF 99101H are at least as potent as sumatriptan and 5-HT, at activating prejunctional inhibitory ca-5-HT1D/1B heteroreceptors on sympathetic axon terminals in dog saphenous vein. In addition, when measured simultaneously in the same tissue preparation,

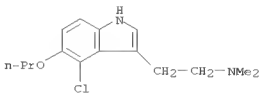
L11 ANSWER 101 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
[3H]noradrenaline release was inhibited to a much greater extent than neurogenic contraction by any particular agonist.

IT 172378-03-9, SKF 99101H
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(measurement of [3H]noradrenaline release and neurogenic contraction to determine the inhibitory effects of SKF 99101H and BRL 56905 in dog vein)

RN 172378-03-9 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-propoxy-, (2E)-2-butenedioate (2:1) (CA INDEX NAME)

CM 1

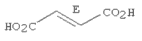
CRN 147405-43-4
CMF C15 H21 Cl N2 O



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

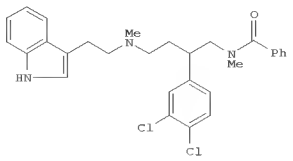


L11 ANSWER 102 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:121333 CAPLUS
DOCUMENT NUMBER: 126:131380
ORIGINAL REFERENCE NO.: 126:25381a
TITLE: Preparation of N-(indoylazaakyl)arylamides and analogs as neurokinin antagonists
INVENTOR(S): McCormick, Kevin D.; Lupo, Andrew T., Jr.
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9639383	A1	19961212	WO 1996-US7960	19960604
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2223239	A1	19961212	CA 1996-2223239	19960604
AU 9659511	A	19961224	AU 1996-59511	19960604
EP 848706	A1	19980624	EP 1996-916750	19960604
EP 848706	B1	20030205		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, LT, LV, FI				
JP 11506736	T	19990615	JP 1996-500829	19960604
AT 232201	T	20030215	AT 1996-916750	19960604
ES 2191755	T3	20030916	ES 1996-916750	19960604
PRIORITY APPLN. INFO.:			US 1995-469315 A	19950606
			WO 1996-US7960 W	19960604

OTHER SOURCE(S): MARPAT 126:131380
GI

L11 ANSWER 102 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



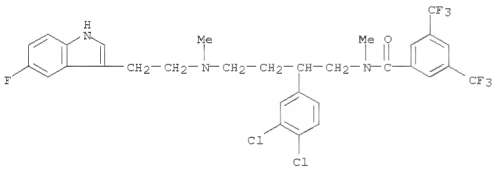
II

AB R(CR5R6)rZ(CR7R8)sCR1R2Z1Z2Z3R3 [I; R = e.g., 3-indolyl; R1 = H, alkyl, (un)substituted Ph, etc.; R2 = (un)substituted (hetero)aryl; R3 = (un)substituted cycloalkyl, -aryl, -heterocyclyl; R5R7 = H, alkyl, CF3, C2F5, (un)substituted Ph, -CH2Ph; R6R8 = groups cited for R5, amino(alkyl), alkoxy(alkyl), etc.; Z = bond, O, CO, (alkyl)imino, CH2, etc.; Z1 = bond, alkylene, CHR2, etc.; Z2 = bond, O, SO0-2, (alkyl)imino, etc.; Z3 = bond, (un)substituted CH2; r,s = 1-4] were prepared Thus, MeNO2 was added to MeO2CCH:CHC6H3Cl3-3,4 to give, after reduction and protection, Me3CMe2SiOCH2CH2CH(CHNH2)C6H3Cl2-3,4 followed by amidation, N-methylation, deprotection, and O-mesylation to give MeSO2OCH2CH2CH(CHNMeBz)C6H3Cl2-3,4. The latter was aminated by N-methyltryptamine to give title compound II. Data for biol. activity of I were given.

IT 186310-14-5P 186310-23-6P 186310-24-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(indoylazaakyl)arylamides and analogs as neurokinin antagonists)

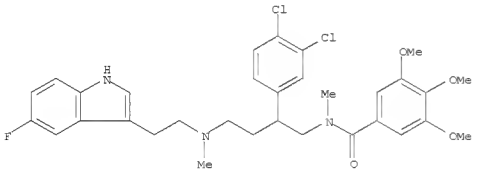
RN 186310-14-5 CAPLUS
CN Benzamide, N-[2-(3,4-dichlorophenyl)-4-[[2-(5-fluoro-1H-indol-3-yl)ethyl]methylamino]butyl]-N-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

L11 ANSWER 102 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



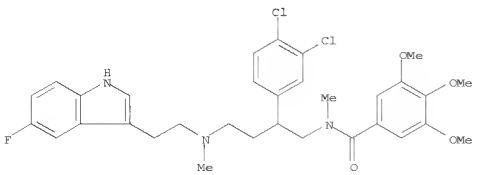
RN 186310-23-6 CAPLUS
CN Benzamide, N-[2-(3,4-dichlorophenyl)-4-[[2-(5-fluoro-1H-indol-3-yl)ethyl]methylamino]butyl]-3,4,5-trimethoxy-N-methyl-, (-)- (CA INDEX NAME)

Rotation (-).



RN 186310-24-7 CAPLUS
CN Benzamide, N-[2-(3,4-dichlorophenyl)-4-[[2-(5-fluoro-1H-indol-3-yl)ethyl]methylamino]butyl]-3,4,5-trimethoxy-N-methyl-, (+)- (CA INDEX NAME)

Rotation (+).

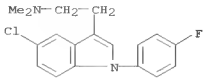


L11 ANSWER 102 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

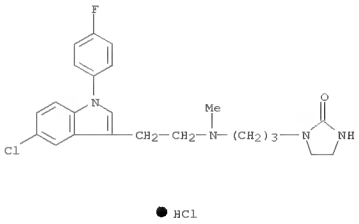
L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:513504 CAPLUS
DOCUMENT NUMBER: 125:195346
ORIGINAL REFERENCE NO.: 125:36583a,36586a
TITLE: Serotonin 5-HT2 Receptor, Dopamine D2 Receptor, and α1 Adrenoceptor Antagonists. Conformationally Flexible Analogs of the Atypical Antipsychotic Sertindole
AUTHOR(S): Andersen, Kim; Perregaard, Jens; Liljefors, Tommy; Hyttel, John
CORPORATE SOURCE: Research Department, H. Lundbeck A/S, Copenhagen, DK-2500, Den.
SOURCE: Journal of Medicinal Chemistry (1996), 39(19), 3723-3738
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Conformationally flexible analogs of the atypical antipsychotic sertindole

(1-[2-[4-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]-4-piperidinyl]ethyl]-2-imidazolidinone) were synthesized. Replacement of the 4-piperidinyl ring in sertindole by a 2-(methylamino)ethoxy group or a 2-(methylamino)ethyl group (e.g. 1-[2-[2-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yloxy]ethylmethylamino]ethyl]-2-imidazolidinone and 1-[3-[[2-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]propyl]-2-imidazolidinone results in binding affinities for serotonin 5-HT2A and dopamine D2 receptors, as well as α1 adrenoceptors, which are very similar to those of sertindole. (Methylamino)alkyl groups of other chain lengths, 3-(methylamino)propyloxy groups, and 2-(methylamino)ethylsulfanyl groups, do not have such properties. The capability of the 2-(methylamino)ethoxy group and the 2-(methylamino)ethyl group to replace the 4-piperidinyl ring in sertindole is reflected in mol. modeling studies using recently published receptor-interaction models for 5-HT2 and D2 receptors. Structure-affinity investigations concerning the substituents in the indole nucleus and the 2-imidazolidinone ring system in the 2-(methylamino)ethoxy and the 2-(methylamino)ethyl analogs of sertindole have led to high affinity serotonin 5-HT2A receptor antagonists with selectivity vs. dopamine D2 receptors and α1 adrenoceptors (e.g. 1-[2-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yloxy]ethyl]methylamino]ethyl]-2-imidazolidinone and 1-[3-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]propyl]-2-imidazolidinone). The latter derivative has also high selectivity for 5-HT2A receptors vs. serotonin 5-HT2C receptors. Replacement of the basic amino group by nitrogen-containing six-membered rings has led to 5-chloro-1-(4-fluorophenyl)-3-[(4-methylpiperazinyl)ethoxy]-1H-indole, which has high affinity for dopamine D2, vs. low affinity for serotonin 5-HT2A receptors and α1 adrenoceptors.
IT 170232-02-7P

L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of conformationally flexible analogs of sertindole as serotonin 5-HT2 receptor, dopamine D2 receptor, and α1 adrenoceptor antagonists)
RN 170232-02-7 CAPLUS
CN 1H-Indole-3-ethanamine, 5-chloro-1-(4-fluorophenyl)-N,N-dimethyl- (CA INDEX NAME)



IT 170231-80-8P 170231-82-0P 170232-03-8P 181115-91-3P 181115-94-6P 181115-96-8P 181115-98-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of conformationally flexible analogs of sertindole as serotonin 5-HT2 receptor, dopamine D2 receptor, and α1 adrenoceptor antagonists)
RN 170231-80-8 CAPLUS
CN 2-Imidazolidinone, 1-[3-[[2-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

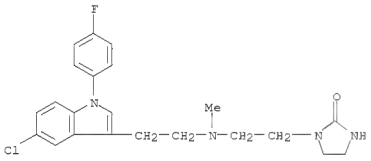


● HCl

L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 170231-82-0 CAPLUS
CN 2-Imidazolidinone, 1-[2-[[2-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]ethyl]-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

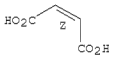
CRN 170231-81-9
CMF C22 H24 Cl F N4 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

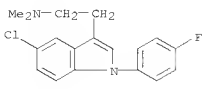
Double bond geometry as shown.



RN 170232-03-8 CAPLUS
CN 1H-Indole-3-ethanamine, 5-chloro-1-(4-fluorophenyl)-N,N-dimethyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

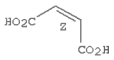
CRN 170232-02-7
CMF C18 H18 Cl F N2



CM 2

L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CRN 110-16-7
CMF C4 H4 O4

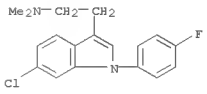
Double bond geometry as shown.



RN 181115-91-3 CAPLUS
CN 1H-Indole-3-ethanamine, 6-chloro-1-(4-fluorophenyl)-N,N-dimethyl-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 181115-90-2
CMF C18 H18 Cl F N2

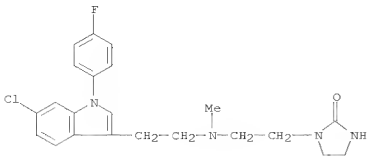


CM 2

CRN 144-62-7
CMF C2 H2 O4

RN 181115-94-6 CAPLUS
CN 2-Imidazolidinone, 1-[2-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

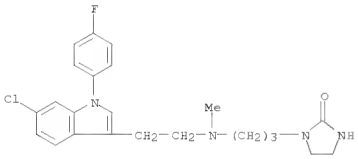


● HCl

RN 181115-96-8 CAPLUS
CN 2-Imidazolidinone, 1-[3-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]propyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 181115-95-7
CMF C23 H26 Cl F N4 O



CM 2

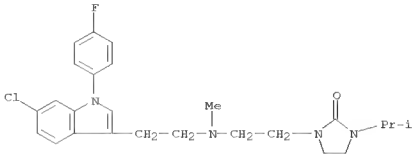
CRN 144-62-7
CMF C2 H2 O4

RN 181115-98-0 CAPLUS

L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN 2-Imidazolidinone, 1-[2-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]ethyl]-3-(1-methylethyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 181115-97-9
CMF C25 H30 Cl F N4 O

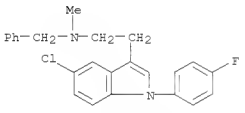


CM 2

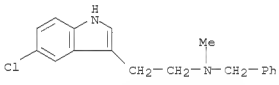
CRN 144-62-7
CMF C2 H2 O4

IT 170232-30-1P 170232-32-3P 181115-88-8P
181115-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of conformationally flexible analogs of sertindole as serotonin
5-HT2 receptor, dopamine D2 receptor, and α1 adrenoceptor antagonists)
RN 170232-30-1 CAPLUS
CN 1H-Indole-3-ethanamine, 5-chloro-1-(4-fluorophenyl)-N-methyl-N-(phenylmethyl)- (CA INDEX NAME)

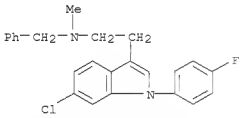
L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



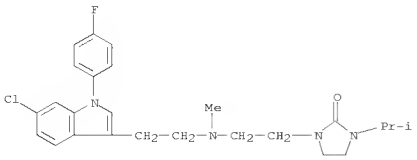
RN 170232-32-3 CAPLUS
CN 1H-Indole-3-ethanamine, 5-chloro-N-methyl-N-(phenylmethyl)- (CA INDEX NAME)



RN 181115-88-8 CAPLUS
CN 1H-Indole-3-ethanamine, 6-chloro-1-(4-fluorophenyl)-N-methyl-N-(phenylmethyl)- (CA INDEX NAME)



RN 181115-97-9 CAPLUS
CN 2-Imidazolidinone, 1-[2-[[2-[6-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]ethyl]methylamino]ethyl]-3-(1-methylethyl)- (CA INDEX NAME)



L11 ANSWER 103 OF 229 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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=> d his

     (FILE 'HOME' ENTERED AT 17:19:21 ON 24 JUN 2008)

     FILE 'REGISTRY' ENTERED AT 17:19:37 ON 24 JUN 2008
L1             STRUCTURE UPLOADED
L2          35 S L1
L3        6038 S L1 FULL
L4             STRUCTURE UPLOADED
L5         275 S L4 FULL  SUB=L3
L6        5763 S L3 NOT L5
L7             STRUCTURE UPLOADED
L8           0 S L7 FULL  SUB=L6
L9             STRUCTURE UPLOADED
L10       1320 S L9 FULL  SUB=L6

     FILE 'CAPLUS' ENTERED AT 17:24:22 ON 24 JUN 2008
L11        229 S L10

=> fil reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                  ENTRY    SESSION
FULL ESTIMATED COST                               55.43     363.52

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                  ENTRY    SESSION
CA SUBSCRIBER PRICE                               -5.60      -5.60

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DICTIONARY FILE UPDATES:  23 JUN 2008  HIGHEST RN 1030103-54-8

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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

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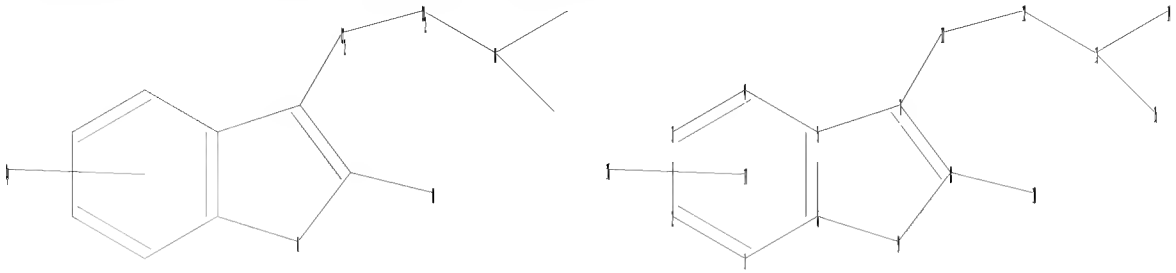

chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom

L12 STRUCTURE UPLOADED

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L12 HAS NO ANSWERS
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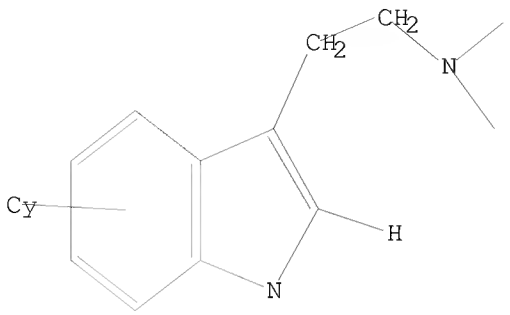

Structure attributes must be viewed using STN Express query preparation.

=> S L12 FULL SUB=L6
FULL SUBSET SEARCH INITIATED 17:46:38 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 5763 TO ITERATE

100.0% PROCESSED 5763 ITERATIONS 21 ANSWERS
SEARCH TIME: 00.00.01

L13 21 SEA SUB=L6 SSS FUL L12

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	42.56	406.08

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.60

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FILE LAST UPDATED: 23 Jun 2008 (20080623/ED)

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http://www.cas.org/legal/infopolicy.html

=> S L13
L14 3 L13

=> D IBIB TOT

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

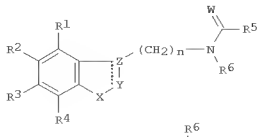
ACCESSION NUMBER: 1997:247954 CAPLUS
DOCUMENT NUMBER: 126:225161
ORIGINAL REFERENCE NO.: 126:43539a,43542a
TITLE: Acylated derivatives of melatonin and its analogs, useful as medicaments
INVENTOR(S): Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacquesy, Jean-Claude; Jouannetaud, Marie-Paule; Violeau, Bruno; Karam, Omar
PATENT ASSIGNEE(S): Cemaf, Fr.; Laboratoires Besins Iscovesco S.A.; Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacquesy, Jean-Claude; Jouannetaud, Marie-Paule; Violeau, Bruno; Karam, Omar
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9706140	A1	19970220	WO 1996-FR1260	19960807
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2737725	A1	19970214	FR 1995-9611	19950808
FR 2737725	B1	19971031		
AU 9668236	A	19970305	AU 1996-68236	19960807
EP 851855	A1	19980708	EP 1996-928490	19960807
EP 851855	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1196049	A	19981014	CN 1996-196943	19960807
CN 1118451	B	20030820		
JP 11510804	T	19990921	JP 1996-508184	19960807
AT 218547	T	20020615	AT 1996-928490	19960807
PT 851855	T	20021031	PT 1996-928490	19960807
ES 2176480	T3	20021201	ES 1996-928490	19960807
JP 4061658	B2	20080319	JP 1997-508184	19960807
ZA 9606751	A	19971103	ZA 1996-6751	19960808
US 6004991	A	19991221	US 1998-11042	19980327
US 6140372	A	20001031	US 1999-292968	19990416

PRIORITY APPLN. INFO.: FR 1995-9611 A 19950808
WO 1996-FR1260 W 19960807

OTHER SOURCE(S): CASREACT 126:225161; MARPAT 126:225161
GI

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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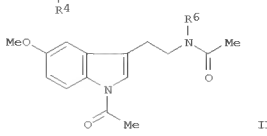


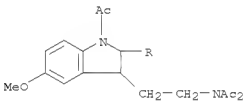
II

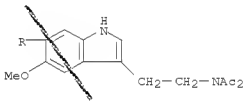
AB Title derivs. I [W = O, S, (un)substituted NH; X = (un)substituted NH, CH:CH, CH2CH2; YZ = CH:C, C(W)CH, CH2CH; or XYZ = (un)substituted CH2CH:CHCH, CH2C(W)CH2CH, CH2CH2C(W)CH; n = 1-4, especially 2; R1-R6 = H, OH, (un)substituted alk(en/yn)yl, cycloalkyl, alkoxy, aryloxy, aralkoxy, alkylthio, halo, NO2, aryl, etc.], are disclosed, as is a method for their preparation, their therapeutic use, particularly for treating diseases associated with melatonin disorders, and pharmaceutical and cosmetic compns. containing them. For example, treatment of melatonin with NaH in THF, followed by acetyl chloride, gave title compds. II [R6 = H and Ac]. Tests in fish showed that I have a hypnotic effect greater than that of melatonin, and equivalent to that of diazepam.

IT 188397-12-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acylated melatonin derivs. as drugs and cosmetics)

RN 188397-12-8 CAPLUS
CN Acetamide, N,N'-[(1-acetyl-2,3-dihydro-5,5'-dimethoxy[2,6'-bi-1H-indole]-3,3'-diyl)di-2,1-ethanediyl]bis[N-acetyl- (9CI) (CA INDEX NAME)

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)





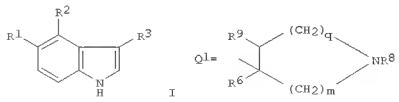
L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:557092 CAPLUS
DOCUMENT NUMBER: 122:290709
ORIGINAL REFERENCE NO.: 122:52999a,53002a
TITLE: Preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists.
INVENTOR(S): Porter, Roderick Alan; Coates, William John
PATENT ASSIGNEE(S): SmithKline Beecham PLC, UK
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9414771	A1	19940707	WO 1993-EP3564	19931214
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9458119	A	19940719	AU 1994-58119	19931214
EP 674620	A1	19951004	EP 1994-903794	19931214
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 08504786	T	19960521	JP 1993-514774	19931214
ZA 9309456	A	19950619	ZA 1993-9456	19931217
CN 1092765	A	19940928	CN 1993-112761	19931220

PRIORITY APPLN. INFO.: GB 1992-26537 A 19921221
WO 1993-EP3564 W 19931214

OTHER SOURCE(S): MARPAT 122:290709
GI



I

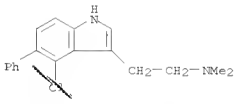
AB Title compds. [I; R1 = (substituted) 6-10-membered (hetero)aryl ring; R2 = H, halo, C1-4 alkyl, CN, NO2, CF3; R3 = CR4R5CH2NR6R7, CH:NNHC(NH)NH2, Q1; R4-R7 = H, C1-4 alkyl; NR6R7 = ring; R8 = H, C1-4 alkyl, C3-6 alkenyl; Ra = H; Rb = H, OH; RaRb = bond; q, m = 1, 2], were prepared I are 5-HT1-like agonists or partial agonists and may be useful in the treatment and/or prophylaxis of migraine, cluster headache, headache associated with vascular

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

disorders and other neuralgia. They are also expected to have utility in the treatment or prophylaxis of portal hypertension. Thus, 2-chloro-6-nitro-3-phenyltoluene (prepn. given) was heated with DMF di-Me acetal and pyrrolidine in DMF at 120°; the resulting eneamine was stirred with N2H4 and Raney Ni in MeOH to give 4-chloro-5-phenylindole. This was stirred with AcCl and bis(dimethylamino)methane in CH2Cl2 to give a residue which was stirred with KCN and MeI in DMF to give 4-chloro-3-cyanomethyl-5-phenylindole. The latter in MeOH was shaken with Me2NH and Raney Ni under 40 psi H to give 4-chloro-3-[2-N,N-(dimethylamino)ethyl]-5-phenylindole. I showed EC50 = 0.03-1.5 μM in the rabbit basilar artery 5-HT1-like receptor screen.

IT 163104-46-9P 163104-47-0P 163104-66-3P
163104-70-9P 163104-71-0P 163104-85-6P
163104-86-7P 163104-89-0P 163104-90-3P
163105-04-2P 163105-07-5P 163105-08-6P
163105-11-1P 163105-26-8P 163105-27-9P
163105-29-1P 163105-95-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)

RN 163104-46-9 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-phenyl- (CA INDEX NAME)

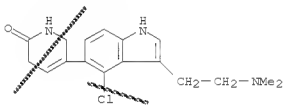


RN 163104-47-0 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-phenyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

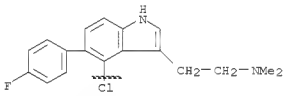
CRN 163104-46-9
CMF C18 H19 Cl N2

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HI

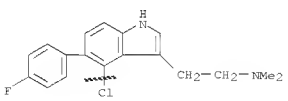
RN 163104-85-6 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl- (CA INDEX NAME)



RN 163104-86-7 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

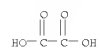
CM 1

CRN 163104-85-6
CMF C18 H18 Cl F N2

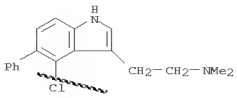


CM 2

CRN 144-62-7
CMF C2 H2 O4



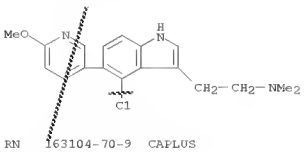
L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



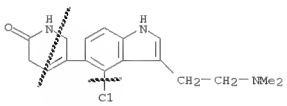
CM 2

CRN 144-62-7
CMF C2 H2 O4

RN 163104-66-3 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(6-methoxy-3-pyridinyl)-N,N-dimethyl- (CA INDEX NAME)



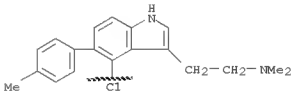
RN 163104-70-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-3,6-dihydro- (CA INDEX NAME)



RN 163104-71-0 CAPLUS
CN 2(1H)-Pyridinone, 5-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-3,6-dihydro-, monohydriodide (9CI) (CA INDEX NAME)

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

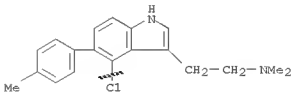
RN 163104-89-0 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)- (CA INDEX NAME)



RN 163104-90-3 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-89-0
CMF C19 H21 Cl N2

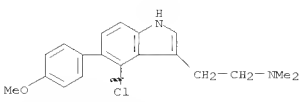


CM 2

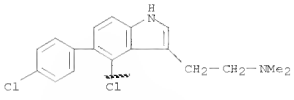
CRN 144-62-7
CMF C2 H2 O4

RN 163105-04-2 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-methoxyphenyl)-N,N-dimethyl- (CA INDEX NAME)

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



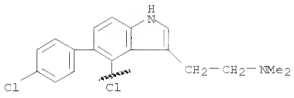
RN 163105-07-5 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl- (CA INDEX NAME)



RN 163105-08-6 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163105-07-5
CMF C18 H18 Cl2 N2

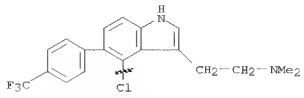


CM 2

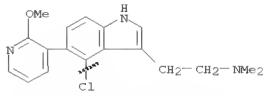
CRN 144-62-7
CMF C2 H2 O4

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

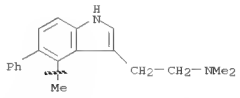
RN 163105-11-1 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 163105-26-8 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(2-methoxy-3-pyridinyl)-N,N-dimethyl- (CA INDEX NAME)



RN 163105-27-9 CAPLUS
CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl- (CA INDEX NAME)

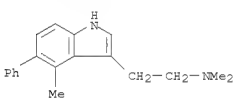


RN 163105-29-1 CAPLUS
CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl-, ethanedioate (9CI) (CA
INDEX NAME)

CM 1

CRN 163105-27-9
CMF C19 H22 N2

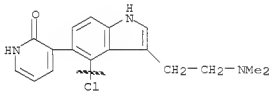
L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



CM 2

CRN 144-62-7
CMF C2 H2 O4

RN 163105-95-1 CAPLUS
CN 2(1H)-Pyridinone, 3-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]- (CA INDEX NAME)

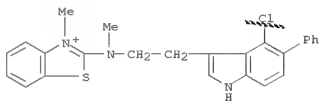


IT 163105-78-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)
RN 163105-78-0 CAPLUS
CN Benzothiazolium, 2-[[2-(4-chloro-5-phenyl-1H-indol-3-yl)ethyl]methylamino]-3-methyl-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

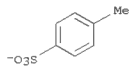
CRN 163105-77-9
CMF C25 H23 Cl N3 S

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



CM 2

CRN 16722-51-3
CMF C7 H7 O3 S



L14 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:187197 CAPLUS
DOCUMENT NUMBER: 90:187197
ORIGINAL REFERENCE NO.: 90:29756h,29757a
TITLE: Quadrigemines-A and -B, two minor alkaloids of Hodgkinsonia frutescens F. Muell
AUTHOR(S): Parry, Keith P.; Smith, George F.
CORPORATE SOURCE: Dep. Chem., Univ. Manchester, Manchester, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (12), 1671-82
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The structures of quadrigemines A [an approx. 1:1 mixture of diastereoisomer I and one (or a mixture of both) of the meso diastereoisomers] and B (II), isolated from H. frutescens leaves, were determined by spectroscopic and chemical means. These are the 1st examples of alkaloid structures made up of 4 tryptamine units.
IT 69937-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69937-12-8 CAPLUS
CN [3,7'-Bi-1H-indole]-3,3'(2H)-diethanamine, N,N,N',N'-tetramethyl-5,5'-dinitro- (9CI) (CA INDEX NAME)